

Unified Description of Dirac Electrons on a Curved Surface of Topological Insulators

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Existence of a protected surface state described by a massless Dirac equation is a defining property of the topological insulator. Though this statement can be explicitly verified on an idealized flat surface, it remains to be addressed to what extent it could be general. On a curved surface, the surface Dirac equation is modified by the spin connection terms. Here, in the light of the differential geometry, we give a general framework for constructing the surface Dirac equation starting from the Hamiltonian for bulk topological insulators. The obtained unified description clarifies the physical meaning of the spin connection.

I. INTRODUCTION

The emergence of low-energy electron states on the surface of a three-dimensional (3D) strong topological insulator is topologically protected by a nontrivial value of the strong \mathbb{Z}_2 index (i.e., $\mathbb{Z}_2 = 1$).^{1–3} These states on a flat surface obey a massless Dirac equation, and possess a linear energy dispersion forming a gapless cone-like structure (i.e., Dirac cone) in reciprocal space. The existence of a single Dirac cone has been verified experimentally by a number of angle-resolved photoemission spectroscopy measurements performed in different realizations of the 3D topological insulator^{4–8} and is now incontrovertible.⁹ It should be noted that these features of Dirac electrons manifest themselves on the flat surface of topological insulator samples. There arises a natural question: how do low-energy electrons behave on a curved surface? The closed surface of any realistic topological insulator sample is inevitably curved, and we expect that this curved nature plays a role in some cases.

The behavior of low-energy electrons on a curved surface of, such as, cylindrical and spherical topological insulators^{10–20} is of considerable theoretical interest. The case of a cylindrical topological insulator^{11–14,16,19} has been studied by the use of an appropriate Dirac equation. A remarkable feature is the appearance of a finite-size energy gap separating the upper and lower Dirac cones of surface electron states. This is the consequence of half-integral quantization of angular momentum caused by a Berry's phase π . The origin of the Berry's phase has been explained as follows: since the real spin of surface electrons is locked on the tangential plane at any point on a curved surface (i.e., spin-to-surface locking), surface curvature induces a Berry's phase π on going around the cylindrical surface. It has been pointed out that the same type of the Berry's phase π appears in the spherical case, and therefore a finite-size energy gap also appears.^{10,15,18}

In spite of the accumulation of such studies, we have so far not reached the unified theoretical framework for analyzing the behavior of the low-energy electrons on a curved surface. It is believed that low-energy states are inevitably described by a Dirac-type equation even on curved surfaces. However, an explicit demonstration of this has been lacking. We here briefly summarize

the present status of the theoretical studies focusing on curved surfaces of topological insulators. The analyses on this problem have been so far performed mainly for cylindrical and spherical systems, to which the following two approaches have been applied. The first group of studies is based on the two-dimensional (2D) Dirac equation for a flat surface, and takes account of the curved nature of the surface by a coordinate transformation.^{10–15} Certainly, the resulting curved surface Dirac theory can be applicable to an arbitrary curved surface in this approach, but for a clear reason that it assumes a 2D Dirac theory from the outset, it fails to answer the question whether the low-energy electrons on an arbitrary curved surface obey indeed a Dirac-type equation. Furthermore, this has a drawback that it ignores the 3D nature of the original problem. In the second category of approaches one starts from a 3D bulk Hamiltonian, and an effective 2D theory for a given curved surface is derived by the use of the $\mathbf{k} \cdot \mathbf{p}$ approximation.^{16–20} This can in principle take account of the 3D nature. In this paper we generalize the second approach and construct a unified framework for analyzing the curved surface problem of topological insulators.

Construction of the general framework reveals the following issues related to the curved surface Dirac theory. One is an insufficiency of the argument on the Berry's phase π . The Berry's phase π is recognized as a consequence of the so-called spin-to-surface locking in literatures.^{11–14,16} However, since this locking breaks down, for example, in spherical topological insulators,¹⁸ the argument based on the spin-to-surface locking is not more than a phenomenological interpretation. Indeed, the appearance of the Berry's phase π should be attributed to something more fundamental. Another issue to be addressed concerns how one should interpret the spin connection in the curved Dirac theory. An effective Hamiltonian in the curved Dirac theory contains a fictitious vector potential that is often referred to as the “spin connection”. The spin connection is a mathematically well-defined concept, and encodes the information on the curved nature of the surface. Yet, its physical origin remains mysterious, at least for those researchers in the condensed matter community. Here, in this paper we attempt an accessible presentation of this issue.

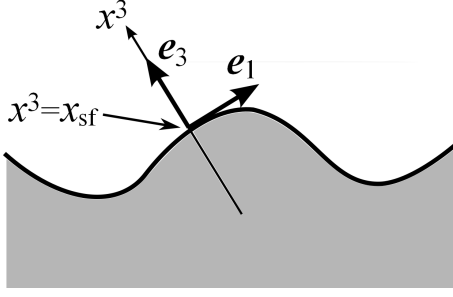


FIG. 1. Curved surface of a 3D topological insulator: cross section in the plane spanned by \mathbf{e}_1 and \mathbf{e}_2 .

In the next section we present a 3D model Hamiltonian for a strong topological insulator and define a set of curvilinear coordinates that can be used to describe an arbitrary curved surface. In §3, we introduce a general framework to derive the effective surface Hamiltonian for the low-energy electrons within the $\mathbf{k} \cdot \mathbf{p}$ approximation. We show that the effective Hamiltonian is indeed expressed in a generalized Dirac form with the spin connection. The role of the spin connection is clarified and given an intuitive interpretation. In §4, we discuss the boundary condition for a spinor wave function in spatially periodic systems, and identify the precise origin of the Berry's phase π . In §5, our framework is applied to two known examples to demonstrate how it works. The last section is devoted to summary and discussion. We set $\hbar = 1$ throughout this paper.

II. MODEL

Let us start with the following bulk effective Hamiltonian for a 3D isotropic (strong) topological insulator in the continuum limit:^{21,22} $H_{\text{bulk}} = m(\mathbf{p})\tau_z + A\tau_x(\boldsymbol{\sigma} \cdot \mathbf{p})$, where $\mathbf{p} = -i\nabla$ and $m(\mathbf{p}) = m_0 + m_2\mathbf{p}^2$ is the mass term. Without loss of generality, we assume that $m_0 > 0$ and $m_2 < 0$. The two types of Pauli matrices $\boldsymbol{\sigma} = (\sigma_x, \sigma_y, \sigma_z)$ and $\boldsymbol{\tau} = (\tau_x, \tau_y, \tau_z)$, respectively, represent the real and orbital spin degrees of freedom. If the ordinary matrix representation of $\boldsymbol{\tau}$ is used, H_{bulk} is expressed as

$$H_{\text{bulk}} = \begin{bmatrix} m(\mathbf{p}) & A(\boldsymbol{\sigma} \cdot \mathbf{p}) \\ A(\boldsymbol{\sigma} \cdot \mathbf{p}) & -m(\mathbf{p}) \end{bmatrix}. \quad (1)$$

Let us consider a curved surface of the sample described by two coordinates (x^1, x^2) as $\mathbf{X}^\alpha = f^\alpha(x^1, x^2)$, where $\mathbf{X} = (X^1, X^2, X^3)$ represents the position of an arbitrary point on the surface in the 3D Cartesian coordinates (see Fig. 1). Depending on the geometry (e.g., closed vs. open surfaces, etc.), the coordinate x_i represents either a linear (non-cyclic) or a cyclic coordinate.

For simplicity we focus on samples whose entire surface is described by a single set of functions $\{f^\alpha\}$, although with little modification our argument can be extended to cases where the entire surface is wrapped by several patches and a separate set of functions is needed to describe each patch. We introduce a curvilinear coordinate system which is suitable to analyze low-energy electron states of the topological insulator localized near its surface. It should be noted that as surface electron states has a finite penetration depth λ , we require that a curvilinear coordinate system is well-defined only in the surface region of width on the order of λ . Let \mathbf{e}_1 and \mathbf{e}_2 be the two tangent vectors defined by

$$\mathbf{e}_i = \frac{\partial \mathbf{X}}{\partial x^i}. \quad (2)$$

Note that \mathbf{e}_1 and \mathbf{e}_2 are not necessarily orthogonal with each other nor normalized to be unity. Let \mathbf{e}_3 be the unit normal vector defined by

$$\mathbf{e}_3 = \frac{\mathbf{e}_1 \times \mathbf{e}_2}{|\mathbf{e}_1 \times \mathbf{e}_2|}, \quad (3)$$

which for simplicity is assumed to be outward normal to the surface. We introduce the third (perpendicular) coordinate x^3 along the straight line designated by \mathbf{e}_3 , and set $x^3 = x_{\text{sf}}$ just on the surface. Let us consider fictitious internal surfaces obtained by varying (x^1, x^2) at fixed values of x^3 satisfying $x_{\text{sf}} \geq x^3 \gtrsim x_{\text{sf}} - \lambda$. These surfaces are well-defined over the entire sample as long as the smallest value of local radius of curvature at $x^3 = x_{\text{sf}}$ is much longer than λ . Let $f^\alpha(x^1, x^2, x^3)$ be the function that describes the internal surface at x^3 . In terms of this we define \mathbf{e}_1 and \mathbf{e}_2 similar to eq. (2). Now \mathbf{e}_1 and \mathbf{e}_2 become functions of (x^1, x^2, x^3) , while \mathbf{e}_3 is independent of x^3 . We employ (x^1, x^2, x^3) as the curvilinear coordinates with the basis vectors

$$\mathbf{e}_1 = \mathbf{e}_1(x^1, x^2, x^3), \quad (4)$$

$$\mathbf{e}_2 = \mathbf{e}_2(x^1, x^2, x^3), \quad (5)$$

$$\mathbf{e}_3 = \mathbf{e}_3(x^1, x^2). \quad (6)$$

Let us introduce \mathbf{e}^i that satisfies $\mathbf{e}_i \cdot \mathbf{e}^j = \delta_{ij}$. We also introduce the metric tensors in a symmetric bilinear form defined by $g_{ij} \equiv \mathbf{e}_i \cdot \mathbf{e}_j$ and $g^{ij} \equiv \mathbf{e}^i \cdot \mathbf{e}^j$, which satisfy $g_{ik}g^{kj} = \delta_{ij}$. Here and hereafter we use the convention that a repeated index, such as i, j , and k , should be summed over 1, 2, 3. Obviously, $g_{33} = g^{33} = 1$ as $|\mathbf{e}_3| = 1$, and $g_{13} = g_{23} = g^{13} = g^{23} = 0$ as $\mathbf{e}_1 \perp \mathbf{e}_3$ and $\mathbf{e}_2 \perp \mathbf{e}_3$. In this coordinate system, an infinitesimal volume element is given by $dV = dS dx^3$ with

$$dS = \sqrt{\mathcal{G}} dx^1 dx^2 \quad (7)$$

being an infinitesimal area element, where

$$\mathcal{G}(x^1, x^2, x^3) \equiv \det\{g_{ij}\} = g_{11}g_{22} - g_{12}^2. \quad (8)$$

Within the curvilinear coordinates presented above, the 3D Cartesian coordinates $(X^1, X^2, X^3) = (x, y, z)$ and

the differential operators with respect to them are represented as $X^\alpha = e_{i\alpha}x^i$ and $\partial/\partial X^\alpha = e^i_\alpha \partial_i$, where $\partial_i \equiv \partial/\partial x^i$. For later convenience we decompose the Laplacian into two parts as $\nabla^2 = \Lambda_\perp + \Lambda_\parallel$, where

$$\Lambda_\perp = \frac{1}{\sqrt{g}} \partial_3 \left(\sqrt{g} \partial_3 \right), \quad (9)$$

$$\Lambda_\parallel = \sum_{i,j=1}^2 \frac{1}{\sqrt{g}} \partial_i \left(\sqrt{g} g^{ij} \partial_j \right). \quad (10)$$

Finally we present a set of equations which describe the spatial variation of \mathbf{e}_i against x^1 and x^2 . The tangent vectors obey the Gauss equation,

$$\partial_j \mathbf{e}_i = \sum_{k=1}^2 \Gamma_{ij}^k \mathbf{e}_k + b_{ij} \mathbf{e}_3, \quad (11)$$

where

$$b_{ij} = -(\partial_j \mathbf{e}_3) \cdot \mathbf{e}_i, \quad (12)$$

$$\Gamma_{ij}^k = \frac{1}{2} g^{kl} (\partial_j g_{li} + \partial_i g_{lj} - \partial_l g_{ij}). \quad (13)$$

The unit normal vector obeys the Weingarten equation,

$$\partial_j \mathbf{e}_3 = - \sum_{i=1}^2 b_j^i \mathbf{e}_i, \quad (14)$$

where

$$b_j^i = \sum_{k=1}^2 g^{ik} b_{kj} = -(\partial_j \mathbf{e}_3) \cdot \mathbf{e}^i. \quad (15)$$

These equations are used in Appendices B and C in deriving, or simplifying, matrix elements of the effective Hamiltonian.

III. DERIVATION OF THE EFFECTIVE HAMILTONIAN

Let us now derive the effective surface Hamiltonian for low-energy electron states of the topological insulator for which curvilinear coordinates (x^1, x^2, x^3) are defined. The derivation consists of four steps.

In the first step, we rewrite eq. (1) in terms of the curvilinear coordinates, and then divide it into perpendicular and parallel components; the former describes the penetration of surface wave functions into the bulk while the latter determines low-energy properties of surface states. As a result, H_{bulk} is decomposed as $H_{\text{bulk}} = H_\perp + H_\parallel$ with

$$H_\perp = \begin{bmatrix} m_0 - m_2 \Lambda_\perp & -iA\sigma^3 \partial_3 \\ -iA\sigma^3 \partial_3 & -m_0 + m_2 \Lambda_\perp \end{bmatrix}, \quad (16)$$

$$H_\parallel = \begin{bmatrix} -m_2 \Lambda_\parallel & -iA \sum_{i=1}^2 \sigma^i \partial_i \\ -iA \sum_{i=1}^2 \sigma^i \partial_i & m_2 \Lambda_\parallel \end{bmatrix}, \quad (17)$$

where we have used $\boldsymbol{\sigma} \cdot \nabla = \sigma^i \cdot \partial_i$ with

$$\sigma^i \equiv \mathbf{e}^i \cdot \boldsymbol{\sigma}. \quad (18)$$

In the second step we solve the perpendicular eigenvalue equation $H_\perp |\psi\rangle = E_\perp |\psi\rangle$,^{16,18,21,22} and obtain two basis states. The appropriate boundary condition for $|\psi\rangle$ is $|\psi(x^3 = x_{\text{sf}})\rangle = \mathbf{0}$. That is, all four components of the wave function $|\psi\rangle$ vanish on the surface at $x^3 = x_{\text{sf}}$. As the simplest approximation, we replace Λ_\perp in H_\perp with

$$\begin{aligned} \Lambda_\perp &= \partial_3^2 + \frac{1}{2} \langle \partial_3 \ln g \rangle \partial_3 \\ &\equiv \partial_3^2 + \Delta(x^1, x^2) \partial_3, \end{aligned} \quad (19)$$

where the definition of the average $\langle \dots \rangle$ over x^3 is given below [see eq. (33)]. Then, we can show that the eigenvalue equation has surface solutions of the damped form, $|\psi\rangle = e^{\kappa(x^3 - x_{\text{sf}})} |u\rangle$. Here κ characterizing the penetration depth λ is determined by $\det\{M_\perp\} = 0$ with

$$M_\perp = \begin{bmatrix} m_0 - m_2 \zeta - E_\perp & -iA\kappa\sigma^3 \\ -iA\kappa\sigma^3 & -m_0 + m_2 \zeta - E_\perp \end{bmatrix}, \quad (20)$$

where $\zeta = \kappa^2 + \Delta\kappa$. Let us introduce the two eigenvectors \mathbf{n}_\pm of σ^3 . They satisfy

$$\sigma^3 \mathbf{n}_\pm = \pm \mathbf{n}_\pm, \quad (21)$$

and are regarded as local spin quantization axis. It should be stressed that \mathbf{n}_\pm points in the $\pm \mathbf{e}_3$ direction if the spin axes (s_x, s_y, s_z) are identified with the 3D Cartesian coordinates (x, y, z) . That is, \mathbf{n}_+ (\mathbf{n}_-) is outward (inward) normal to the tangential plane at (x^1, x^2) on the surface. In terms of the 4×4 unitary matrix U defined by $U = \text{diag}\{u, u\}$ with $u = (\mathbf{n}_+, \mathbf{n}_-)$, we can diagonalize M_\perp as

$$U^\dagger M_\perp U = \begin{bmatrix} m_0 - m_2 \zeta - E_\perp & -iA\kappa\sigma_z \\ -iA\kappa\sigma_z & -m_0 + m_2 \zeta - E_\perp \end{bmatrix}. \quad (22)$$

Now we can easily show that

$$\det\{M_\perp\} = [E_\perp^2 + (A\kappa)^2 - (m_0 - m_2 \zeta)^2]^2 = 0. \quad (23)$$

This indicates that there exist doubly degenerate four different values of κ . Two of which are evanescent solutions (i.e., $\kappa > 0$) exponentially damped deep inside the sample, while the other two correspond to exponentially increasing solutions. By superposing two evanescent solutions with $\kappa = \kappa_\pm$, we construct a general solution localized near the surface as

$$|\psi\rangle = e^{\kappa_-(x^3 - x_{\text{sf}})} |u_-\rangle - e^{\kappa_+(x^3 - x_{\text{sf}})} |u_+\rangle. \quad (24)$$

The boundary condition $|\psi(x^3 = x_{\text{sf}})\rangle = \mathbf{0}$ holds only when $|u_+\rangle = |u_-\rangle$ for $\kappa_+ \neq \kappa_-$. As shown in Appendix A, we see that this results in the zero-energy condition $E_\perp = 0$ and

$$\kappa_\pm(x^1, x^2) = \frac{A \pm \sqrt{A^2 + 4m_0 m_2}}{-2m_2} \quad (25)$$

with $\mathcal{A} \equiv A + m_2 \Delta$. We also find that two basis eigenstates, $|+\rangle$ and $|-\rangle$, for H_\perp with $E_\perp = 0$ are given by

$$|\pm\rangle(x^1, x^2, x^3) = \rho(x^3; x^1, x^2)|\pm\rangle(x^1, x^2) \quad (26)$$

with

$$|\pm\rangle(x^1, x^2) = \frac{1}{\sqrt{2}} \begin{bmatrix} \mathbf{n}_+ \\ \mp i \mathbf{n}_- \end{bmatrix} \quad (27)$$

and

$$\rho(x^3; x^1, x^2) = \frac{1}{\sqrt{c}} \left(e^{\kappa_-(x^3 - x_{\text{sf}})} - e^{\kappa_+(x^3 - x_{\text{sf}})} \right), \quad (28)$$

where $c(x^1, x^2)$ is a normalization constant. The x^1 - and x^2 -dependences of ρ arise from c and κ_\pm .

In the third step we derive the effective surface Hamiltonian within the $\mathbf{k} \cdot \mathbf{p}$ -approximation. The following derivation is based on the observation that any surface state $|\Psi\rangle$ can be represented as a linear combination of $|+\rangle$ and $|-\rangle$ with the amplitude respectively specified by $\tilde{\alpha}_+$ and $\tilde{\alpha}_-$, i.e.,

$$|\Psi\rangle = \tilde{\alpha}_+ |+\rangle + \tilde{\alpha}_- |-\rangle. \quad (29)$$

Within the $\mathbf{k} \cdot \mathbf{p}$ -approximation, the effective surface Hamiltonian $\tilde{\mathcal{H}}_{\text{eff}}$ for the two-component spinor $\tilde{\alpha} = {}^t(\tilde{\alpha}_+, \tilde{\alpha}_-)$ is given by

$$\tilde{\mathcal{H}}_{\text{eff}} = \begin{bmatrix} \langle + | H_\parallel | + \rangle & \langle + | H_\parallel | - \rangle \\ \langle - | H_\parallel | + \rangle & \langle - | H_\parallel | - \rangle \end{bmatrix}. \quad (30)$$

Here, each matrix element is expressed by

$$\langle \sigma | H_\parallel | \sigma' \rangle = \int_{x_{\text{sf}} - l_c}^{x_{\text{sf}}} dx^3 \sqrt{\mathcal{G}} \rho \langle \sigma | H_\parallel | \sigma' \rangle \rho, \quad (31)$$

where l_c is the cutoff length being much longer than the penetration depth λ . Note that the factor $\sqrt{\mathcal{G}}$ reflects the fact that $dV = \sqrt{\mathcal{G}} dx^1 dx^2 dx^3$. Accordingly, we set the normalization constant as

$$c(x^1, x^2) = \int_{x_{\text{sf}} - l_c}^{x_{\text{sf}}} dx^3 \sqrt{\mathcal{G}} \left(e^{\kappa_-(x^3 - x_{\text{sf}})} - e^{\kappa_+(x^3 - x_{\text{sf}})} \right)^2. \quad (32)$$

Hereafter we use the shorthand notation of the average over x^3 defined by

$$\langle \dots \rangle = \frac{\int_{x_{\text{sf}} - l_c}^{x_{\text{sf}}} dx^3 \dots \rho^2}{\int_{x_{\text{sf}} - l_c}^{x_{\text{sf}}} dx^3 \rho^2}. \quad (33)$$

The average in eq. (19) should be identified with this.

Without loss of generality we hereafter require that \mathbf{n}_\pm are connected by time-reversal operation as

$$\mathbf{n}_+ = -i\sigma_y \mathbf{n}_-^*, \quad (34)$$

indicating that if $\mathbf{n}_- = {}^t(n_1, -n_2)$, then $\mathbf{n}_+^\dagger = (n_2, n_1)$. If \mathbf{e}^3 is parameterized in terms of spherical coordinates $\theta(x^1, x^2)$ and $\phi(x^1, x^2)$ as $\mathbf{e}^3 = (\sin \theta \cos \phi, \sin \theta \sin \phi, \cos \theta)$ and hence

$$\sigma^3 = \begin{bmatrix} \cos \theta & \sin \theta e^{-i\phi} \\ \sin \theta e^{i\phi} & -\cos \theta \end{bmatrix}, \quad (35)$$

a natural solution of eq. (21) is given by

$$\mathbf{n}_+(x^1, x^2) = \begin{bmatrix} \cos \frac{\theta}{2} e^{-i\frac{\phi}{2}} \\ \sin \frac{\theta}{2} e^{i\frac{\phi}{2}} \end{bmatrix}, \quad (36)$$

$$\mathbf{n}_-(x^1, x^2) = \begin{bmatrix} \sin \frac{\theta}{2} e^{-i\frac{\phi}{2}} \\ -\cos \frac{\theta}{2} e^{i\frac{\phi}{2}} \end{bmatrix}. \quad (37)$$

This standard expression of \mathbf{n}_\pm obviously satisfies eq. (34). Note that in the derivation of the effective surface Hamiltonian, we require only eq. (34) and do not explicitly use eqs. (36) and (37).

Let us evaluate the matrix elements given in eq. (31). We easily find that the diagonal elements vanish, i.e., $\langle \pm | H_\parallel | \pm \rangle = 0$. In evaluating the off-diagonal elements, we should note that ∂_i in H_\parallel acts on not only $|\pm\rangle(x^1, x^2)$ but also $\rho(x^3; x^1, x^2)$. After straightforward calculations (see Appendix B), we find

$$\tilde{\mathcal{H}}_{\text{eff}} = \begin{bmatrix} 0 & \tilde{D}_+ \\ \tilde{D}_- & 0 \end{bmatrix} \quad (38)$$

with

$$\tilde{D}_+ = \sum_{i=1}^2 \left[(\eta_i A - \xi_i m_2) \partial_i + \frac{1}{2} [\partial_i (\eta_i A - \xi_i m_2)] \right], \quad (39)$$

$$\tilde{D}_- = \sum_{i=1}^2 \left[-(\eta_i A - \xi_i m_2)^* \partial_i - \frac{1}{2} [\partial_i (\eta_i A - \xi_i m_2)^*] \right], \quad (40)$$

where

$$\begin{aligned} \eta_i &= \int_{x_{\text{sf}} - l_c}^{x_{\text{sf}}} dx^3 \sqrt{\mathcal{G}} \rho^2 \mathbf{n}_+^\dagger \sigma^i \mathbf{n}_- \\ &= \frac{\langle \sqrt{\mathcal{G}} \mathbf{n}_+^\dagger \sigma^i \mathbf{n}_- \rangle}{\langle \sqrt{\mathcal{G}} \rangle}, \end{aligned} \quad (41)$$

$$\begin{aligned} \xi_i &= 2 \sum_{j=1}^2 \int_{x_{\text{sf}} - l_c}^{x_{\text{sf}}} dx^3 \sqrt{\mathcal{G}} \rho^2 g^{ij} \mathbf{n}_+^\dagger \partial_j \mathbf{n}_- \\ &= 2 \sum_{j=1}^2 \frac{\langle \sqrt{\mathcal{G}} g^{ij} \mathbf{n}_+^\dagger \partial_j \mathbf{n}_- \rangle}{\langle \sqrt{\mathcal{G}} \rangle}. \end{aligned} \quad (42)$$

We show in Appendix C that ξ_i is simplified to

$$\xi_i = \sum_{j=1}^2 \frac{\langle \sqrt{\mathcal{G}} b_j^i \mathbf{n}_+^\dagger \sigma^j \mathbf{n}_- \rangle}{\langle \sqrt{\mathcal{G}} \rangle}, \quad (43)$$

where $b_j^i = -(\partial_j \mathbf{e}_3) \cdot \mathbf{e}^i$. The second term in $\tilde{\mathcal{D}}_{\pm}$ is essential in ensuring the hermiticity of $\tilde{\mathcal{H}}_{\text{eff}}$ when the coefficient $\eta_i A - \xi_i m_2$ depends on x^i .^{17,23,24} It should be noted that the effective velocity in the x^i -direction is determined by $\eta_i A - \xi_i m_2$, where the second term with m_2 represents the renormalization due to curvature.^{17,20}

In the final step we slightly modify the obtained effective Hamiltonian to adapt our framework to the standard convention. Since we insert the factor $\sqrt{\mathcal{G}}$ in the definition of the matrix elements [see eq (31)], the integral measure for the orthonormalization of $\tilde{\alpha}$ is $dx^1 dx^2$. However, $d\langle S \rangle \equiv \langle \sqrt{\mathcal{G}} \rangle dx^1 dx^2$ is a more natural choice. Accordingly we define the new two-component spinor α as

$$\alpha \equiv \frac{1}{\sqrt{\langle \sqrt{\mathcal{G}} \rangle}} \tilde{\alpha}, \quad (44)$$

for which $d\langle S \rangle$ can be applied. The effective Hamiltonian for α is obtained as

$$\mathcal{H}_{\text{eff}} = \begin{bmatrix} 0 & \mathcal{D}_+ \\ \mathcal{D}_- & 0 \end{bmatrix}, \quad (45)$$

where

$$\begin{aligned} \mathcal{D}_+ = \sum_{i=1}^2 \left[(\eta_i A - \xi_i m_2) \left(\partial_i + \frac{1}{2} \left[\partial_i \ln \langle \sqrt{\mathcal{G}} \rangle \right] \right) \right. \\ \left. + \frac{1}{2} [\partial_i (\eta_i A - \xi_i m_2)] \right], \end{aligned} \quad (46)$$

$$\begin{aligned} \mathcal{D}_- = \sum_{i=1}^2 \left[-(\eta_i A - \xi_i m_2)^* \left(\partial_i + \frac{1}{2} \left[\partial_i \ln \langle \sqrt{\mathcal{G}} \rangle \right] \right) \right. \\ \left. - \frac{1}{2} [\partial_i (\eta_i A - \xi_i m_2)^*] \right]. \end{aligned} \quad (47)$$

The above set of equations, eq. (45) with eqs. (46) and (47), constitutes the central result of the paper.

We have thus seen that the obtained effective Hamiltonian takes indeed a generalized Dirac form with linear differential operators. Low-energy electrons on the arbitrary curved surface of a topological insulator do obey a Dirac equation. It should be also emphasized that the obtained linear differential operator involves a correction term, $(1/2)\partial_i \ln \langle \sqrt{\mathcal{G}} \rangle$, that corresponds precisely to what is known as the spin connection in the Dirac theory on curved surfaces.^{10–12,15,25} By noting $d\langle S \rangle = \langle \sqrt{\mathcal{G}} \rangle dx^1 dx^2$, we have identified the precise origin of the spin connection as arising from the spatial variations of an infinitesimal area element. Last but not the least, we have pointed out that the last term in the expression for \mathcal{D}_{\pm} [see eqs. (46) and (47)] appears for ensuring the hermiticity of \mathcal{H}_{eff} , and is unrelated to the spin connection itself.

IV. ORIGIN OF THE BERRY'S PHASE π

Let us discuss the origin of the Berry's Phase π in the context of the boundary condition for $\alpha(x^1, x^2) =$

${}^t(\alpha_+, \alpha_-)$, and its relation to the so-called spin-to-surface locking. Let us consider a situation in which either one or both of our curvilinear coordinates x^i are *cyclic*. Angular coordinates of a closed (e.g., cylindrical or spherical) geometry could be a typical example of such a coordinate. In the following we assume that only the coordinate x^i ($i = 1$ or 2) is cyclic with a cycle of L_i (the other coordinate does not appear explicitly in the discussion). Our starting point is the fact that any wave function

$$|\Psi(x^i)\rangle = \alpha_+(x^i)|+\rangle(x^i) + \alpha_-(x^i)|-\rangle(x^i) \quad (48)$$

must satisfy the periodic boundary condition, i.e.,

$$|\Psi(x^i)\rangle = |\Psi(x^i + L_i)\rangle. \quad (49)$$

The local spin quantization axis $\mathbf{n}_{\pm}(x^i)$ plays a crucial role in our argument. Obviously, if $\mathbf{n}_{\pm}(x^i) = \mathbf{n}_{\pm}(x^i + L_i)$ and hence $|\pm\rangle(x^i) = |\pm\rangle(x^i + L_i)$, the boundary condition for $\alpha(x^i)$ must be periodic as

$$\alpha(x^i) = \alpha(x^i + L_i). \quad (50)$$

Note that \mathbf{n}_{\pm} could change its sign as $\mathbf{n}_{\pm}(x^i) = -\mathbf{n}_{\pm}(x^i + L_i)$ after the coordinate x^i finishes one complete cycle of evolution (i.e., $x^i \rightarrow x^i + L_i$). If this is the case, the sign of $|\pm\rangle(x^i)$ is also reversed as $|\pm\rangle(x^i) = -|\pm\rangle(x^i + L_i)$. Accordingly, the boundary condition for α must be antiperiodic as

$$\alpha(x^i) = -\alpha(x^i + L_i). \quad (51)$$

This indicates that the boundary condition for α is simply determined by whether or not $\mathbf{n}_{\pm}(x^i)$ changes its sign when the cyclic coordinate x^i is shifted by one complete cycle L_i (in geometrical terms, this would correspond to one complete revolution of the Dirac electron around the closed surface). Actually, $\mathbf{n}_{\pm}(x^i)$ changes its sign when it *rotates* by $\pm 2\pi$ around an arbitrary axis in the spin space as the Dirac electron *revolves* once around the closed surface.

Let us observe that the antiperiodicity of the boundary condition discussed above is equivalent to the Berry's phase π in the Dirac theory on curved surfaces. In the latter point of view the antiperiodic boundary condition is abandoned (i.e., replaced with the periodic one) at the cost of introducing a Berry's phase π . This can be seen as follows: we focus on the case in which \mathbf{n}_{\pm} changes its sign as $\mathbf{n}_{\pm}(x^i) = -\mathbf{n}_{\pm}(x^i + L_i)$. Then, we reformulate this problem by the use of the following single-valued basis vectors

$$\tilde{\mathbf{n}}_{\pm}(x_i) \equiv \exp\left(i\pi \frac{x_i}{L_i}\right) \mathbf{n}_{\pm}(x_i), \quad (52)$$

which obviously satisfy the periodic boundary condition: $\tilde{\mathbf{n}}_{\pm}(x^i) = \tilde{\mathbf{n}}_{\pm}(x^i + L_i)$. Reflecting the fact that eq. (34) does not hold for $\tilde{\mathbf{n}}_{\pm}$, the effective Hamiltonian in this single-valued basis becomes

$$\mathcal{H}_{\text{eff}}^{\text{sv}} = \begin{bmatrix} 0 & \mathcal{D}_+^{\text{sv}} \\ \mathcal{D}_-^{\text{sv}} & 0 \end{bmatrix}, \quad (53)$$

where

$$\mathcal{D}_+^{\text{sv}} = \sum_{i=1}^2 \left[(\eta_i A - \xi_i m_2) \left(\partial_i + \frac{1}{2} [\partial_i \ln \langle \sqrt{\mathcal{G}} \rangle] + i \frac{\pi}{L_i} \right) + \frac{1}{2} [\partial_i (\eta_i A - \xi_i m_2)] \right], \quad (54)$$

$$\mathcal{D}_-^{\text{sv}} = \sum_{i=1}^2 \left[-(\eta_i A - \xi_i m_2)^* \left(\partial_i + \frac{1}{2} [\partial_i \ln \langle \sqrt{\mathcal{G}} \rangle] + i \frac{\pi}{L_i} \right) - \frac{1}{2} [\partial_i (\eta_i A - \xi_i m_2)^*] \right]. \quad (55)$$

Note that in the above formulas the change of the boundary condition has been absorbed as a correction to derivatives, i.e., the term of the form of $i\pi/L_i$, which sums up to a Berry's phase π . In this sense, the Berry's phase π is a mere rewriting of the antiperiodicity of the basis vectors \mathbf{n}_\pm , while it is often regarded as an important part of the spin connection in literatures.^{11,12,16,18}

We have so far argued that the Berry's phase π should be attributed to the sign change of the local spin quantization axis \mathbf{n}_\pm caused by a $\pm 2\pi$ rotation in the spin space. Previously, the Berry's phase π is interpreted as a consequence of the spin-to-surface locking.^{11-14,16} This statement is plausible, but fails to capture the precise origin of this term. Indeed, even in the situation where the Berry's phase π or equivalently the antiperiodic boundary condition plays a role, the spin-to-surface locking does not necessarily or globally occur, as is demonstrated in the spherical system of a topological insulator.¹⁸ The Berry's phase π is encoded in the surface Dirac theory, specified by an explicit form of the effective surface Hamiltonian and by the periodicity of the boundary condition of \mathbf{n}_\pm as well. Contrastingly, the spin-to-surface locking is not an ingredient of the surface Dirac theory but a characteristic feature of the typical surface wave functions, and in this sense not appropriate for being given a full status as the *origin* of the Berry's phase π .

V. APPLICATION TO REPRESENTATIVE CASES

In this section we apply the general framework established so far to the following two representative cases: samples of either a cylindrical or a spherical shape and find an explicit formula [corresponding to eqs. (46) and (47)] of the differential operators \mathcal{D}_\pm that specify the explicit form of the Dirac Hamiltonian (45). In the analysis given below we employ orthogonal curvilinear coordinates, for which $g_{ij} = \text{diag}(g_{11}, g_{22}, 1)$ and $g^{ij} = \text{diag}(g^{11}, g^{22}, 1)$ with $g^{11} = (g_{11})^{-1}$ and $g^{22} = (g_{22})^{-1}$.

A. The cylindrical case

Let us consider an infinitely long cylindrical topological insulator aligned along the z -axis with radius R .

We employ the following three coordinates $(x^1, x^2, x^3) = (\phi, z, r)$, in terms of which the 3D Cartesian coordinates are expressed as $(x, y, z) = (r \cos \phi, r \sin \phi, z)$. The parameter x_{sf} is simply equal to R . The tangent and normal vectors are

$$\mathbf{e}_1 = (-r \sin \phi, r \cos \phi, 0), \quad (56)$$

$$\mathbf{e}_2 = (0, 0, 1), \quad (57)$$

$$\mathbf{e}_3 = (\cos \phi, \sin \phi, 0), \quad (58)$$

and

$$\mathbf{e}^1 = \left(-\frac{\sin \phi}{r}, \frac{\cos \phi}{r}, 0 \right), \quad (59)$$

$$\mathbf{e}^2 = (0, 0, 1), \quad (60)$$

$$\mathbf{e}^3 = (\cos \phi, \sin \phi, 0). \quad (61)$$

The elements of the metric tensors are $g_{11} = r^2$ and $g_{22} = 1$, which results in $\mathcal{G} = r^2$, and the coefficients of the Weingarten equation are $b_1^1 = -r^{-1}$ and $b_1^2 = b_2^1 = b_2^2 = 0$. From the expressions of \mathbf{e}^i we obtain the spin matrices as

$$\sigma^1 = \frac{i}{r} \begin{bmatrix} 0 & -e^{-i\phi} \\ e^{i\phi} & 0 \end{bmatrix}, \quad (62)$$

$$\sigma^2 = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}, \quad (63)$$

$$\sigma^3 = \begin{bmatrix} 0 & e^{-i\phi} \\ e^{i\phi} & 0 \end{bmatrix}. \quad (64)$$

As the unit vectors satisfying $\sigma^3 \mathbf{n}_\pm = \pm \mathbf{n}_\pm$, it is convenient to use those given in eqs. (36) and (37) at $\theta = \pi/2$,

$$\mathbf{n}_\pm = \frac{1}{\sqrt{2}} \begin{bmatrix} e^{-i\frac{\phi}{2}} \\ \pm e^{i\frac{\phi}{2}} \end{bmatrix}. \quad (65)$$

Then we immediately find that $\mathbf{n}_+^\dagger \sigma^1 \mathbf{n}_- = ir^{-1}$ and $\mathbf{n}_+^\dagger \sigma^2 \mathbf{n}_- = 1$. Substitution of these results with $\sqrt{\mathcal{G}} = r$ and $b_1^1 = -r^{-1}$ and $b_1^2 = b_2^1 = b_2^2 = 0$ into eqs. (41) and (43) yields

$$\eta_1 = \frac{\langle ir^{-1} \sqrt{\mathcal{G}} \rangle}{\langle \sqrt{\mathcal{G}} \rangle} = \frac{i}{\langle r \rangle}, \quad (66)$$

$$\eta_2 = 1, \quad (67)$$

$$\xi_1 = \frac{-\langle ir^{-2} \sqrt{\mathcal{G}} \rangle}{\langle \sqrt{\mathcal{G}} \rangle} = -\frac{i}{\langle r \rangle} \left\langle \frac{1}{r} \right\rangle, \quad (68)$$

$$\xi_2 = 0. \quad (69)$$

Noting that $\partial_\phi \ln \langle \sqrt{\mathcal{G}} \rangle = \partial_z \ln \langle \sqrt{\mathcal{G}} \rangle = 0$ we finally obtain the differential operator \mathcal{D}_\pm as

$$\mathcal{D}_\pm = i \left(A + \left\langle \frac{1}{r} \right\rangle m_2 \right) \frac{\partial_\phi}{\langle r \rangle} \pm A \partial_z. \quad (70)$$

If the penetration depth λ for surface states is much shorter than R , we can approximate as $\langle r \rangle = R$ and $\langle r^{-1} \rangle = R^{-1}$, and then \mathcal{D}_\pm is simplified to

$$\mathcal{D}_\pm = i \left(A + \frac{m_2}{R} \right) \frac{\partial_\phi}{R} \pm A \partial_z. \quad (71)$$

The effective Hamiltonian is given by eq. (45) with \mathcal{D}_\pm obtained above. The result similar to this has been reported in ref.¹⁶, where the renormalization correction m_2/R to the effective velocity is ignored. Let us consider the boundary condition for a spinor wave function $\alpha(\phi, z)$. Since $\mathbf{n}_\pm(\phi)$ in eq. (65) changes its sign when $\phi \rightarrow \phi + 2\pi$, the boundary condition for the variable ϕ must be antiperiodic, i.e.,

$$\alpha(\phi, z) = -\alpha(\phi + 2\pi, z). \quad (72)$$

B. The spherical case

We turn to the second case of a spherical topological insulator with radius R . We employ the standard spherical coordinates $(x^1, x^2, x^3) = (\theta, \phi, r)$, in terms of which the 3D Cartesian coordinates are expressed as $(x, y, z) = (r \sin \theta \cos \phi, r \sin \theta \sin \phi, r \cos \theta)$. The parameter x_{sf} is again equal to R . The tangent and normal vectors are

$$\mathbf{e}_1 = (r \cos \theta \cos \phi, r \cos \theta \sin \phi, -r \sin \theta), \quad (73)$$

$$\mathbf{e}_2 = (-r \sin \theta \sin \phi, r \sin \theta \cos \phi, 0), \quad (74)$$

$$\mathbf{e}_3 = (\sin \theta \cos \phi, \sin \theta \sin \phi, \cos \theta), \quad (75)$$

and

$$\mathbf{e}^1 = \left(\frac{\cos \theta \cos \phi}{r}, \frac{\cos \theta \sin \phi}{r}, -\frac{\sin \theta}{r} \right), \quad (76)$$

$$\mathbf{e}^2 = \left(-\frac{\sin \phi}{r \sin \theta}, \frac{\cos \phi}{r \sin \theta}, 0 \right), \quad (77)$$

$$\mathbf{e}^3 = (\sin \theta \cos \phi, \sin \theta \sin \phi, \cos \theta). \quad (78)$$

The elements of the metric tensors are $g_{11} = r^2$ and $g_{22} = r^2 \sin^2 \theta$, which results in $\mathcal{G} = r^4 \sin^2 \theta$, and the coefficients of the Weingarten equation are $b_1^1 = b_2^2 = -r^{-1}$, and $b_1^2 = b_2^1 = 0$. From the expressions of \mathbf{e}^i we obtain the spin matrices as

$$\sigma^1 = \frac{1}{r} \begin{bmatrix} -\sin \theta & \cos \theta e^{-i\phi} \\ \cos \theta e^{i\phi} & \sin \theta \end{bmatrix}, \quad (79)$$

$$\sigma^2 = \frac{i}{r \sin \theta} \begin{bmatrix} 0 & -e^{-i\phi} \\ e^{i\phi} & 0 \end{bmatrix}, \quad (80)$$

$$\sigma^3 = \begin{bmatrix} \cos \theta & \sin \theta e^{-i\phi} \\ \sin \theta e^{i\phi} & -\cos \theta \end{bmatrix}. \quad (81)$$

As the unit vectors satisfying $\sigma^3 \mathbf{n}_\pm = \pm \mathbf{n}_\pm$, it is convenient to use those given in eqs. (36) and (37). We find

that $\mathbf{n}_+^\dagger \sigma^1 \mathbf{n}_- = -r^{-1}$ and $\mathbf{n}_+^\dagger \sigma^2 \mathbf{n}_- = i(r \sin \theta)^{-1}$. Substitution of these results with $\sqrt{\mathcal{G}} = r^2 \sin \theta$, $b_1^1 = b_2^2 = -r^{-1}$, and $b_1^2 = b_2^1 = 0$ into eqs. (41) and (43) yields

$$\eta_1 = \frac{-\langle r^{-1} \sqrt{\mathcal{G}} \rangle}{\langle \sqrt{\mathcal{G}} \rangle} = -\frac{\langle r \rangle}{\langle r^2 \rangle}, \quad (82)$$

$$\eta_2 = \frac{i \langle (r \sin \theta)^{-1} \sqrt{\mathcal{G}} \rangle}{\langle \sqrt{\mathcal{G}} \rangle} = \frac{i \langle r \rangle}{\langle r^2 \rangle \sin \theta} \quad (83)$$

$$\xi_1 = \frac{\langle r^{-2} \sqrt{\mathcal{G}} \rangle}{\langle \sqrt{\mathcal{G}} \rangle} = \frac{1}{\langle r^2 \rangle}, \quad (84)$$

$$\xi_2 = \frac{-i \langle (r^2 \sin \theta)^{-1} \sqrt{\mathcal{G}} \rangle}{\langle \sqrt{\mathcal{G}} \rangle} = -\frac{i}{\langle r^2 \rangle \sin \theta}. \quad (85)$$

Noting that $\partial_\theta \ln \langle \sqrt{\mathcal{G}} \rangle = \cot \theta$ and $\partial_\phi \ln \langle \sqrt{\mathcal{G}} \rangle = 0$ we finally obtain the differential operator \mathcal{D}_\pm as

$$\mathcal{D}_\pm = \left(A + \frac{m_2}{\langle r \rangle} \right) \frac{\langle r \rangle}{\langle r^2 \rangle} \left(\mp \partial_\theta + i \frac{\partial_\phi}{\sin \theta} \mp \frac{1}{2} \cot \theta \right). \quad (86)$$

It should be emphasized that $(1/2) \cot \theta$ is identified with the spin connection in the curved Dirac theory.^{15,25} If the penetration depth λ for surface states is much shorter than R , we can approximate as $\langle r \rangle = R$ and $\langle r^2 \rangle = R^2$, and \mathcal{D}_\pm is simplified to

$$\mathcal{D}_\pm = \left(A + \frac{m_2}{R} \right) \frac{1}{R} \left(\mp \partial_\theta + i \frac{\partial_\phi}{\sin \theta} \mp \frac{1}{2} \cot \theta \right). \quad (87)$$

The effective Hamiltonian is given by eq. (45) with \mathcal{D}_\pm obtained above. The result similar to this has been reported in ref.¹⁸, where the renormalization correction m_2/R to the effective velocity is ignored. Let us consider the boundary condition for a spinor wave function $\alpha(\theta, \phi)$. The system is periodic with respect to ϕ , so we consider the boundary condition when ϕ is increased by 2π . Since $\mathbf{n}_\pm(\phi, \theta)$ changes its sign when $\phi \rightarrow \phi + 2\pi$, the boundary condition for the variable ϕ must be antiperiodic, i.e.,

$$\alpha(\theta, \phi) = -\alpha(\theta, \phi + 2\pi). \quad (88)$$

VI. SUMMARY AND DISCUSSION

The behavior of low-energy electrons on an arbitrary curved surface of 3D (strong) topological insulators has been considered on general grounds. In contrast to the specific cases studied earlier, we have reached a unified description of such low-energy electrons by giving the most general form of the surface Dirac Hamiltonian [eq. (45) with eqs. (46) and (47)] that has been explicitly derived from the bulk effective theory in the continuum limit. It was shown that the low-energy surface electrons do obey the Dirac equation in this generalized form with the effective velocity renormalized by the curved nature of the surface. A special attention has been paid to the boundary condition for a spinor wave function α , which

becomes relevant on a closed surface described by at least one *cyclic* coordinate x^i . Whether the boundary condition is periodic or antiperiodic depends on the behavior of the local spin quantization axis \mathbf{n}_\pm . If the sign of \mathbf{n}_\pm is unchanged after one complete cyclic evolution of the coordinate x^i , the boundary condition for α is periodic. On contrary, if \mathbf{n}_\pm changes its sign due to a $\pm 2\pi$ rotation in the spin space, the boundary condition becomes antiperiodic. It is argued that the antiperiodicity of the boundary condition is equivalent to the Berry's phase π .

Previously, the effective Hamiltonian for Dirac electrons on a curved surface has been considered in a framework different from the one presented in this paper.^{10–12,15} In this alternative viewpoint, one starts from a two-dimensional Dirac equation for a flat surface, and takes account of the curved nature of a surface by a coordinate transformation, resulting in the curved surface Dirac theory. The effective Hamiltonian thus obtained contains a fictitious vector potential called the spin connection, which corresponds to the term $(1/2)\partial_i \ln \langle \sqrt{\mathcal{G}} \rangle$ in our framework. We have shown that the spin connection represents corrections arising from the spatial variation of an infinitesimal area element. We have also seen that such an *ad hoc* curved Dirac theory overlooks the renormalization of the effective velocity arising from the quadratic mass term m_2 . This is because the theory ignores from the outset the three dimensional nature of the problem. It should be noted that the above renormalization arises even in the limit in which the penetration depth λ of surface states is vanishingly short, as is seen in §5.

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Appendix A: Proof of $E_\perp = 0$

As noted in the text, the boundary condition $|\psi(x^3 = x_{\text{sf}})\rangle = \mathbf{0}$ holds only when $|u_+\rangle = |u_-\rangle$ for $\kappa_+ \neq \kappa_-$. Here $|u_\pm\rangle$ are the eigenvectors satisfying $M_\perp(\kappa_\pm)|u_\pm\rangle = \mathbf{0}$, where

$$M_\perp(\kappa_\pm) = \begin{bmatrix} m_0 - m_2\zeta_\pm - E_\perp & -iA\kappa_\pm\sigma^3 \\ -iA\kappa_\pm\sigma^3 & -m_0 + m_2\zeta_\pm - E_\perp \end{bmatrix} \quad (\text{A1})$$

with $\zeta_\pm = \kappa_\pm^2 + \Delta\kappa_\pm$. It is instructive to rewrite the eigenvalue equation as

$$\begin{bmatrix} \frac{m_0 - m_2\zeta_\pm - E_\perp}{A\kappa_\pm} & -i\sigma^3 \\ -i\sigma^3 & -\frac{m_0 - m_2\zeta_\pm + E_\perp}{A\kappa_\pm} \end{bmatrix} |u_\pm\rangle = \mathbf{0}. \quad (\text{A2})$$

From the above equation we easily observe that if $|u_+\rangle = |u_-\rangle$, the following two equations

$$\frac{m_0 - m_2\zeta_+ - E_\perp}{A\kappa_+} = \frac{m_0 - m_2\zeta_- - E_\perp}{A\kappa_-}, \quad (\text{A3})$$

$$\frac{m_0 - m_2\zeta_+ + E_\perp}{A\kappa_+} = \frac{m_0 - m_2\zeta_- + E_\perp}{A\kappa_-} \quad (\text{A4})$$

must hold simultaneously. This directly results in $E_\perp = 0$. Under this zero energy condition, $\det\{M_\perp\} = 0$ yields $m_0 - m_2\zeta_\pm = A\kappa_\pm$, where $m_0 > 0$ and $m_2 < 0$ are assumed. Solving $m_0 - m_2\zeta_\pm = A\kappa_\pm$ with respect to κ_\pm , we obtain eq. (25).

Appendix B: Derivation of the Off-Diagonal Matrix Elements

From eqs. (17), (26) and (27) it is easy to show that

$$\langle +|H_\parallel|-\rangle = \int_{x_{\text{sf}}-l_c}^{x_{\text{sf}}} dx^3 \sqrt{\mathcal{G}} \rho \left(A \sum_{i=1}^2 \mathbf{n}_+^\dagger \sigma^i \partial_i \mathbf{n}_- - m_2 \mathbf{n}_+^\dagger \Lambda_\parallel \mathbf{n}_- \right) \rho. \quad (\text{B1})$$

Let us denote the first and second terms in the right-hand side of eq. (B1) as $\langle +|H_\parallel|-\rangle_1$ and $\langle +|H_\parallel|-\rangle_2$, respectively. The first term is rewritten as

$$\langle +|H_\parallel|-\rangle_1 = \sum_{i=1}^2 \left[\eta_i A \partial_i + \frac{1}{2} (\partial_i \eta_i A) + A P_i \right] \quad (\text{B2})$$

where η_i is defined in eq. (41) and

$$P_i = -\frac{1}{2} \int_{x_{\text{sf}}-l_c}^{x_{\text{sf}}} dx^3 \rho^2 \left[\mathbf{n}_+^\dagger (\partial_i \sqrt{\mathcal{G}} \sigma^i) \mathbf{n}_- + \sqrt{\mathcal{G}} \left((\partial_i \mathbf{n}_+^\dagger) \sigma^i \mathbf{n}_- - \mathbf{n}_+^\dagger \sigma^i (\partial_i \mathbf{n}_-) \right) \right]. \quad (\text{B3})$$

We can show $(\partial_i \mathbf{n}_+^\dagger) \sigma^i \mathbf{n}_- - \mathbf{n}_+^\dagger \sigma^i (\partial_i \mathbf{n}_-) = 0$ by using eq. (34), and P_i is reduced to

$$P_i = -\frac{1}{2} \int_{x_{\text{sf}}-l_c}^{x_{\text{sf}}} dx^3 \rho^2 \mathbf{n}_+^\dagger (\partial_i \sqrt{\mathcal{G}} \sigma^i) \mathbf{n}_-. \quad (\text{B4})$$

It is easy to show with $\mathbf{e}^1 = \mathbf{e}_2 \times \mathbf{e}_3 / \sqrt{\mathcal{G}}$ and $\mathbf{e}^2 = \mathbf{e}_3 \times \mathbf{e}_1 / \sqrt{\mathcal{G}}$ that

$$\partial_1 \sqrt{\mathcal{G}} \sigma^1 = [(\partial_1 \mathbf{e}_2) \times \mathbf{e}_3 + \mathbf{e}_2 \times (\partial_1 \mathbf{e}_3)] \cdot \boldsymbol{\sigma}, \quad (\text{B5})$$

$$\partial_2 \sqrt{\mathcal{G}} \sigma^2 = [(\partial_2 \mathbf{e}_3) \times \mathbf{e}_1 + \mathbf{e}_3 \times (\partial_2 \mathbf{e}_1)] \cdot \boldsymbol{\sigma}. \quad (\text{B6})$$

Applying the Gauss equation (11) and the Weingarten equation (14), we find that

$$\partial_1 \sqrt{\mathcal{G}} \sigma^1 = \sqrt{\mathcal{G}} (\Gamma_{21}^2 \sigma^1 - \Gamma_{21}^1 \sigma^2 + b_1^1 \sigma^3), \quad (\text{B7})$$

$$\partial_2 \sqrt{\mathcal{G}} \sigma^2 = \sqrt{\mathcal{G}} (-\Gamma_{12}^2 \sigma^1 + \Gamma_{12}^1 \sigma^2 + b_2^2 \sigma^3). \quad (\text{B8})$$

Substituting these into eq. (B4) and using $\Gamma_{ij}^k = \Gamma_{ji}^k$ and $\mathbf{n}_+^\dagger \sigma^3 \mathbf{n}_- = 0$, we find that $\sum_{i=1}^2 P_i = 0$. Now we turn to the second term which is given by

$$\langle +|H_{||}|-\rangle_2 = -m_2 \sum_{i,j=1}^2 \int_{x_{sf}-l_c}^{x_{sf}} dx^3 \rho \mathbf{n}_+^\dagger \times \partial_i \left(\sqrt{g} g^{ij} \partial_j \right) \mathbf{n}_- \rho. \quad (\text{B9})$$

Since $\mathbf{n}_+^\dagger \mathbf{n}_- = 0$, only the terms with $\mathbf{n}_+^\dagger \partial_i \mathbf{n}_-$ or $\mathbf{n}_+^\dagger \partial_i \partial_j \mathbf{n}_-$ do not vanish. It is then reduced to

$$\langle +|H_{||}|-\rangle_2 = \sum_{i=1}^2 \left[-\xi_i m_2 \partial_i - \frac{1}{2} (\partial_i \xi_i m_2) + m_2 Q_i \right], \quad (\text{B10})$$

where ξ_i is defined in eq. (42) and

$$Q_i = \sum_{j=1}^2 \int_{x_{sf}-l_c}^{x_{sf}} dx^3 \sqrt{g} \rho^2 g^{ij} (\partial_i \mathbf{n}_+^\dagger) (\partial_j \mathbf{n}_-). \quad (\text{B11})$$

We can show with eq. (34) that $\sum_{i,j=1}^2 g^{ij} (\partial_i \mathbf{n}_+^\dagger) (\partial_j \mathbf{n}_-) = 0$. Hence $\sum_{i=1}^2 Q_i = 0$.

Combining the resulting $\langle +|H_{||}|-\rangle_1$ and $\langle +|H_{||}|-\rangle_2$ we finally arrive at eq. (39). The expression of $\langle -|H_{||}|+\rangle$ can also be obtained by repeating the procedure described above.

Appendix C: Simplification of ξ_i

In this short Appendix we simplify the expression of ξ_i defined in eq. (42). The starting point is the following eigenvalue equation: $\sigma^3 \mathbf{n}_- = -\mathbf{n}_-$. Differentiating this by x^j and then constructing the inner product between the resulting expression and \mathbf{n}_+ , we obtain

$$\mathbf{n}_+^\dagger (\partial_j \mathbf{n}_-) = -\frac{1}{2} \mathbf{n}_+^\dagger (\partial_j \sigma^3) \mathbf{n}_-. \quad (\text{C1})$$

The Weingarten equation (14) enables us to replace $\partial_j \sigma^3 = (\partial_j \mathbf{e}^3) \cdot \boldsymbol{\sigma}$ with $-\sum_{k=1}^2 b_{jk} \sigma^k$. This results in

$$\xi_i = \sum_{j,k=1}^2 \int_{x_{sf}-l_c}^{x_{sf}} dx^3 \sqrt{g} \rho^2 g^{ij} b_{jk} \mathbf{n}_+^\dagger \sigma^k \mathbf{n}_-. \quad (\text{C2})$$

Noting that $\sum_{j=1}^2 g^{ij} b_{jk} = b_k^i$, the expression (C2) for ξ_i is reduced to eq. (43).

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